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Ely M. Gelbard

Applied Physics Division
Argonne National Laboratory
Argonne, Illinois 60439

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Ely M. Gelbard

Applied Physics Division
Argonne National Laboratory
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This paper surveys the present capabilities and limitations of S_N, Monte Carlo, and finite element transport computational methods. Outstanding problems remaining in these computational methods are discussed.

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INTRODUCTION

The neutron transport computational methods in use today seem to fall naturally into five different classes. Collision probability and transfer matrix methods, which are treated in Leonard's paper (1), constitute two of these classes. Methods in these two categories tend to be very efficient precisely because, in practice, they involve very substantial approximations. In contrast, the Monte Carlo and discrete ordinates methods, and methods based on polynomial expansions, are generally much less efficient (and more expensive), but also more accurate. It is these more or less exact methods which will be discussed here.

DETERMINISTIC METHODS

The earliest, and perhaps the simplest, polynomial expansion method is, of course, the spherical harmonics method. Both the spherical harmonics method and the discrete ordinates method were applied, first, to the slab transport equation and, in slab geometry, these two methods are very closely related. It is only when we deal with more complicated geometries that the discrete ordinate and spherical harmonics methods acquire totally different properties, both from a theoretical and a practical point of view.

There is at least one very important and very striking difference between the discrete ordinate and spherical harmonics equations, a difference in their fundamental properties. The discrete ordinate equations, in effect, constrain the neutrons to move in straight lines, while the spherical harmonics equations do not. This distortion of neutron trajectories in the spherical harmonics method gives rise to some peculiar anomalies and has important consequences.

Imagine, for example, an absorbing sphere of radius R (which will be called "Region I"), embedded in an infinite absorbing medium, a medium in which the scattering cross section is zero. There is a uniform isotropic source in the sphere, but the surrounding region (Region II) is source-free. Suppose we wish to compute the net leakage rate out of the sphere. It is clear on physical grounds that the leakage rate should not depend on the Region II cross section but, in a spherical harmonics approximation of any order, it does. Further, in diffusion theory, we find that the flux in both regions becomes flat, and the leakage rate goes to zero, as Σ_{aII} goes to zero. When the product $\Sigma_{aII}R$ is small, while $\Sigma_{aI}R$ is large, the diffusion approximation grossly underestimates the leakage rate. In the complementary problem, where the source is in Region II and Region I is source-

free then, again when $\Sigma_{aII}R << 1$ and $\Sigma_{aI}R >> 1$, diffusion theory grossly underestimates the *absorption rate* in Region I.

Of course this particular problem configuration is not one which will be met in practice very often but, unfortunately, related anomalies do crop up in *practical* problems. It is sometimes necessary, in reactor analysis, to compute the leakage into a small absorbing lump. If such a lump, with a large macroscopic cross section, is embedded in a material having a much lower cross-section diffusion theory may grossly underestimate the absorption rate in the lump. Further, if the lump is small enough, the sequence of P_L approximations will converge only very slowly to the true absorption rate.

Another well-known weakness of the spherical harmonics methods is their inability to treat streaming in voids. Unless the diffusion coefficient is artificially adjusted the diffusion approximation completely falls apart in voids and, again, the sequence of P_L approximations converges very slowly in such cases.

In certain situations the P_L equations can be approximated very accurately by a simple set of coupled diffusion equations (2,3), and in such situations they are easy to solve. On the other hand, in their exact form, the multidimensional P_L equations become rapidly more complicated as L increases. Computational algorithms for solving the P_L equations tend, therefore, to be complicated, inefficient, and not completely reliable.

Given all the disadvantages of the spherical harmonics method it is not surprising that most of its early supporters and advocates abandoned it some time ago. Until recently the spherical harmonics had been used only rarely in more than one dimension.

But obviously the discrete ordinates method also has weaknesses and, as the use of discrete ordinates codes has become more widespread, these weaknesses have attracted a good deal of attention. Probably the most famous affliction of the discrete ordinates method is the ray effect (4). If an isotropic line source is inserted into an infinite, purely absorbing medium, the scalar flux produced by this source should certainly have azimuthal symmetry. But in a discrete ordinates approximation the neutrons can move only along rays which lie along the ordinates. In the x-y plane then, the scalar flux will be infinite along the x-y projections of each ordinate, and zero elsewhere. Of course in a medium with scattering the flux will be positive everywhere, but noticeable spurious bumps in the flux may remain. There is no such effect in the spherical harmonics method, which has very nice symmetry properties. The spherical harmonics equations are invariant under all rotations of the coordinate axis,

while the discrete ordinates equations are not. After being harassed by ray effects for many years, practitioners of the discrete ordinates method started looking covetously at the spherical harmonics method, even while many disillusioned spherical harmonics specialists were reluctantly switching their allegiance to the S_N method.

It was Lathrop (4,5) who first showed that discrete ordinate codes, slightly modified, could be used to solve "spherical-harmonics-like" equations. Following a suggestion by Carlson, Lathrop added a fictitious source to the S_N equations, a source which was a linear combination of spatial derivatives of the angular fluxes. This source was so defined as to guarantee that a limited number of flux moments would satisfy spherical harmonics equations of some order, L. Lathrop's method required, in principle, that $L \leq N - 3$, where N is the order of the S_N approximation. In practice, it turned out that Lathrop often obtained anomalous results for $L > N/2$.

It is clear that Lathrop's modified S_N equations are not *exactly* equivalent to the sphrical harmonics equations since, for a given problem configuration and a given L, his computed scalar fluxes vary with N. Why this should be true, however, seems not at all clear at this time.

Reed (6) points out that: "In x-y geometry standard S_N quadrature sets involve the use of $1/2[N(N + 2)]$ quadrature points or directions, giving $1/2[N(N + 2)]$ unknown functions to be determined. In this same geometry a P_L solution will involve $1/2[(L + 1)(L + 2)]$ unknown functions." Thus, in Lathrop's method, the number of S_N ordinates is much greater than the number of unknown functions in the "equivalent" spherical harmonics approximations. An alternate method proposed by Reed is somewhat more economical in that the S_N equations are made "equivalent" to the P_L equations with $L = N - 1$. Reed's method also involves a fictitious source (again a linear combination of derivatives of the angular fluxes) but a source which is somewhat different from Lathrop's. Reed notes that, if one is willing to adopt unsymmetric S_N quadrature sets, then it is possible to define the fictitious source in such a way that the modified S_N calculation becomes "equivalent" to a P_L solution with the *same* number of unknown functions. Thus, for example, a three-ordinate set would be required for an $S_N - P_1$ calculation. In work published simultaneously with Reed's, Jung and his coworkers (using methods very much like Reed's) independently developed $S_N - P_L$ equations of this sort (7), i.e. $S_N - P_L$ equations with $1/2[L(L + 1)]$ ordinates, arranged in unsymmetric sets.

To what extent are these various $S_N - P_L$ approximations *really* equivalent to spherical harmonics approximations? The

Reed and Jung S_N - P_L equations are certainly equivalent to true P_L equations at points where the cross sections are continuous. There is, however, no obvious connection between the Rumyantsev (8) interface conditions, generally used in P_L approximations, and the continuity conditions imposed at interfaces in most S_N - P_L codes. Thus, for example, in a P_1 approximation, and in x-y geometry, the x current is a continuous function of x and the y current is continuous in y; but the y current is not always continuous in x. The y current must be discontinuous across any interface parallel to the y axis if D is discontinuous. If D is discontinuous, then it is impossible for a continuous scalar flux and continuous currents to satisfy the P_1 equations. Yet in S_N - P_L codes the angular fluxes *are* generally taken to be continuous across interfaces. The P_L moments are defined to be linear combinations of the angular fluxes, linear combinations with constant coefficients. All moments, it would seem, must then be continuous.

At this time the behavior of S_N - P_L solutions is not clearly understood. It seems likely, however, that if, in an S_N - P_L code, the angular fluxes are forced to be continuous, then they will change very rapidly at interfaces so as to approximate *discontinuous* functions.* Perhaps, as the mesh widths go to zero, the angular fluxes become discontinuous and, correspondingly, the fictitious sources contain δ-function components. In recent work at Los Alamos (11), Miller finds that S_N - P_1 currents do, in fact, appear to satisfy the ordinary P_1 continuity conditions at convergence, but that the convergence rate of the iterative computational process depends strongly on the nature of the spatial difference equations. The diamond-difference equations explicitly force continuity of the angular fluxes at interfaces and, when the diamond equations are used, convergence is very slow. On the other hand, the step equations do not *explicitly* force continuity: when step equations are used convergence is achieved more quickly, though the convergence rate remains much lower than in conventional S_N codes.

At any rate the S_N - P_L approximations *are* free of ray effects (7). In a limited number (and perhaps not enough) tests these approximations seem, in addition, to be fairly accurate. Unfortunately the S_N - P_L calculations are also expensive, partly because the additional source term converges slowly.

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* In fact Jung argues, in recent work (9), that diamond-difference solutions of the S_N - P_L equations converge, in the L_2 norm, to solutions of the corresponding spherical harmonics equations. In his proof, however, it is assumed that the angular flux and its spatial derivatives are continuous in r. Since this is not always true (10) Jung's proof may not be valid, although his conclusions may be correct nevertheless.

The finite element treatment of the angular variables combines, in some degree, various features of the discrete ordinate and spherical harmonics methods. When the finite element method is used to discretize these variables the unit sphere is, generally, subdivided into disjoint subintervals. Within each subinterval, the angular flux is then represented as a polynomial, of some sort, in some function of the angles, but the flux or its angular derivatives may be discontinuous at subinterval boundaries. Thus, the artificial coupling between fluxes in different directions ought to be somewhat weaker than in the spherical harmonics approximations. On the other hand, the coupling between angular fluxes *within* each subinterval should tend to mitigate ray effects.

The finite element method has been used by Ohinishi to discretize the space (12) and angle (13) variables, separately. Miller, Lewis and Rossow (14) discretize both the space and angle variables simultaneously.* Ohnishi's angular basis functions are general polynomials in the direction cosines μ and η. Miller and his colleagues use functions which are bilinear in θ and ϕ. Ohnishi does not report numerical results in Ref. 13, but we see in Ref. 14 that the finite element method *can* eliminate ray effects in problem configurations where S_N ray effects are quite severe.

It is clear, then, that the spherical harmonics method, and associated partial-range polynomial expansions (like the finite element method), have some very attractive features. But, unfortuately, it is still too early to celebrate mankind's total victory over the neutron transport equations. It is important to remember that the spherical harmonics method has not been neglected for so many years simply through an oversight. Multidimensional spherical harmonics computations are still expensive. Solutions of the P_L equations still converge very slowly, in voids and small absorbing lumps, as L increases. At this point it seems that the spherical harmonics method is appropriate only in special situations, as an auxiliary computational technique.

Apparently at least one of the undesirable traits of the spherical harmonics method has been inherited by the finite element method. Because of the complicated coupling between angles in the finite element method the finite element equations take much more time to solve, for a given number of unknowns, than the S_N equations. As for the accuracy of the finite element approximation (when applied to the angle variable) very little information is available. In particular, more data must be accumulated before one can judge the performance of the finite element method

*For other work on phase space finite element methods see also Refs. 15 and 16.

in those situations where the spherical harmonics method displays its disadvantages most conspicuously.

In differencing the transport equation it is necessary to discretize *both* the angular *and* spatial variables. The difficulties involved in differencing the angle variable have been discussed above. Ray effects are a chronic affliction of the S_N method, brought on by conventional angle differencing techniques. Correspondingly the standard S_N *spatial* difference approximations have their own characteristic weaknesses. It is clear that the solution of the neutron transport equation must be positive if the source is positive. For the sake of brevity we will say that the transport equation has "positivity". The S_N spatial difference equations, however, need not have this property. Perversely, those difference equations which tend to be most accurate (in the limit as the mesh widths approach zero) lack positivity (17). One finds, for example, that solutions of the diamond equations (which, when the mesh widths are small, are among the most accurate S_N difference equations available to us) become oscillatory, and may become negative, as the mesh widths increase. On the other hand the step equations, which are less accurate for small mesh widths, yield non-oscillatory, positive, fluxes whenever the source itself is non-oscillatory and positive.

Two different "fixup" techniques have been used in S_N codes to suppress negative fluxes. In some codes the negative fluxes are simply set to zero whenever they occur in the course of the inner iterative process. In others one automatically switches from diamond to step equations, within a mesh box, when it is detected that the diamond equations will generate a negative angular flux at the boundary of that box. In many respects neither technique is wholly satisfactory.

In Ref. 17, Lathrop proposed a set of difference equations (the "weighted-diamond" equations) intermediate in form between the step and the diamond equations. These weighted-diamond equations contained adjustable parameters ("weights") which controlled their properties. For certain extreme values of the weights the proposed equations degenerated completely into the usual step and diamond equations. In practice, the parameters were to be chosen (during execution of the S_N computation) so as to guarantee that the weighted equations would be "close" to the diamond equations whenever possible but would in any case, always yield positive fluxes.

Lathrop, however, has not continued his work on the weighted-diamond scheme, and now prefers the set-to-zero flux fixup which was described earlier. He argues as follows.

In the weighted-diamond computation the weighting parameters are adjusted, within each mesh box, during the mesh sweep, as soon as the fluxes entering that box are know. It is desired that the adjusted equations be as close as possible to the diamond equations (in some sense) but that they be constrained to yield non-negative exiting fluxes. Suppose one of the diamond equations exiting fluxes is negative. Then, by definition, an exiting flux which is non-negative, yet is as close as possible to that particular diamond-difference flux, must be equal to zero. Presumably, then, an optimum choice of the weighting parameters would produce a zero exiting flux in place of the corresponding, negative, diamond-difference flux. The optimum weighted-diamond scheme would, by this argument, be equivalent to the simple set-to-zero flux-fixup algorithm.

But, whatever the merits of this argument, a variant of the weighted-diamond scheme recently developed by Lee (18) seems to show some promise. Fundamentally the Lee and Lathrop weighted-diamond equations are very similar, though Lee's method for setting the adjustable parameters differs substantially from that originally proposed by Lathrop. Lee's method is now used extensively at Los Alamos, but more information on the performance of the method is needed before it can be fully assessed. In particular, more information is needed about the accuracy of the weighted-diamond equations, compared to the accuracy of the ordinary diamond equations with their associated fixup schemes.

For the sake of brevity I shall not attempt, here, a complete survey of recent literature on the finite element method as it has been applied to the spatial variables. I will, however, comment specifically on work by Reed and Hill (19), and by Kaper, Leaf and Lindemann (16), since these authors have reported some particularly interesting test results.

Reed and Hill have experimented with the finite element method, in various forms, in a somewhat specialized triangular mesh. They applied the finite element method only to the spatial variable, retaining the conventional S_N treatment of the angular variable. Within each triangle the angular flux is represented as a polynomial. In one set of finite element approximations the angular fluxes are forced to be continuous across triangle boundaries while, in another set, angular fluxes at these boundaries are allowed to be discontinuous. An analysis of the results of their test computations leads the authors to the following conclusions:

(1) Errors in integrated quantities (i.e. integrated fluxes or reaction rates) are $O(h^2)$, whatever the order of the polynomial basis functions.

(2) Errors in fluxes at points are O(h), whatever the order of the polynomial basis functions.

(3) Oscillations in the flux, and negative fluxes, tend to be strongly suppressed when the flux is allowed to be discontinuous at element interfaces.

Apparently the order of the error in finite element methods, (as they are currently formulated) is limited by singularities in the angular flux, singularities whose presence was first noted by Arkuszewski, Julikowska and Mika (10). On the basis of their test results Reed and Hill concluded that discontinuous ("nonconforming") finite element approximations are superior to confirming approximations. They have, therefore, incorporated a nonconforming approximation into TRIPLET (20), a triangular mesh transport code recently developed at Los Alamos. It is interesting to note that Kaper, Leaf and Lindemann (16), also,have compared the accuracy of finite element computations with conforming and nonconforming elements: they, also, conclude that nonconforming elements seem to be preferable.

The finite element method may be applied to the neutron transport equation either in its first- or second-order form. Thus, for example, work by Ohnishi (12), and by Reed and Hill (19), is based on the first-order form, while Miller and his colleagues (14), as well as Kaper, Leaf and Lindemann (16), treat the second-order form. In a recent paper (21), Briggs, Miller and Lewis show that, when a simple finite element method is applied to the angular variables in the second-order form, the resulting differential equation (in x and y) is elliptic. Since an elliptic equation has no real characteristics, its solution must be free of ray effects. The fact that the second-order form generates such elliptic equations is noted also by Kaper, Leaf and Lindemann (16); but these authors point out that elliptic equations lead to boundary value problems which are, generally, more difficult to solve than initial value problems. Thus, the finite element methods which are most effective in eliminating ray effects are also, from a practical point of view, the most akward and inconvenient methods. It seems reasonable to conclude, from all that has been said here, that conventional S_N codes will be with us for a very long time.

MONTE CARLO METHODS

It is not feasible to undertake, here, a complete review of Monte Carlo methods in all their many forms. Instead we shall sketch, very briefly, the capabilities of methods currently in use, as well as their most serious weaknesses.

The advantages of the Monte Carlo method are well known. First, it is relatively easy to put complicated cross sections, and complicated geometric detail into Monte Carlo codes. To treat such complications by deterministic methods is relatively difficult. Secondly, the only significant unavoidable errors in Monte Carlo (at least in principle) are statistical errors, and the Monte Carlo method can itself (again, at least in principle) provide us with estimates of these errors.

On the other hand we find that, when one fully utilizes all the capabilities of Monte Carlo methods, Monte Carlo computations can be quite expensive. Generally, the more information one demands from any Monte Carlo computation, the greater the cost. Thus, for example, while it is possible to compute Monte Carlo fluxes in a limited number of regions, and even at a limited number of points (22), it is prohibitively expensive (by current Monte Carlo method* to generate a detailed plot of fluxes or reaction rates.

Further it should be understood that Monte Carlo estimates are often biased, and that estimates of statistical errors are not always reliable. Monte Carlo estimates of ratios are almost invariably biased. Eigenvalue computations are always biased (24), and most are not (by Gast's definition (24)) "fair games". In any Monte Carlo calculation where (as in shielding calculations) the sampling distributions are far from normal, it is extremely difficult to estimate realistic error bounds. In principle it is always possible to set *conservative* bounds, through use of Tchebycheff inequality (25), if the variance of the sampling distribution is known. Unfortunately, however, when the sampling distribution is badly skewed, estimates of the variance may be totally misleading so that even the Tchebyscheff inequality is not always helpful.

But even when one deals with distributions which *are* normal the computations of error estimates is not necessarily a simple task. Thus it is very difficult, in many cases, to produce reliable error estimates in eigenvalue problems, simply because sample values obtained from successive generations are correlated (26). The degree of correlation increases with the dominance ratio and, for example, in large thermal reactors, where the dominance ratio may be very close to one, error estimation techniques which ignore these correlations will be grossly inadequate.

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* Detailed flux plots can be obtained by conditional Monte Carlo (23), but very little is known, at present, about the capabilities and limitations of conditional Monte Carlo in neutron transport computations.

Unfortunately the only methods available today for treating such correlations have no firm theoretical foundation.

Of course Monte Carlo codes are not intended primarily for the computation of error estimates. It is not very consoling to know that an error estimate is reliable if the estimated error is intolerably large. Statistical fluctuations are themselves perhaps the most troublesome feature of Monte Carlo, particularly in perturbation calculations. Various Monte Carlo techniques have been developed specifically for the treatment of small perturbations. One (generally attributed to Mathes (27)) involves the estimation of a bilinear functional in the fission source and its adjoint. In order to evaluate this functional Matthes assumes that the source and the adjoint source are flat over prescribed regions. This is, of course, an approximation and, unfortunately, an approximation whose accuracy is difficult to assess. Though the Matthes method in its original form was based on first-order perturbation theory, recent work has shown (28) that the perturbation approximation is not an essential feature of the Matthes method. The method can be reformulated so as to avoid perturbation theory, but unfortunately other weaknesses in the Matthes method remain.

A second method goes by various names, but is often referred to as "complete correlation" (25). The method of complete correlation involves the simultaneous treatment of perturbed and unperturbed problem configurations, using a single set of histories. Complete correlation is an exact method. The use of complete correlation does not necessarily entail *any* special approximation. That the method is exact seems to be its most attractive feature, but it has its share of compensating disadvantages. Complete correlation is most effective when the "perturbed" and "unperturbed" states are physically very similar. On the other hand, it may be very ineffective when these states differ substantially. Consider, for example, two LMFBR reactors which are identical, except in their coolant regions. Suppose that sodium has been voided from certain coolant channels of one reactor, while the second reactor is in its normal state. The net change in eigenvalue caused by coolant voiding may be very small (i.e. $<<1\%$), but the physical properties of the voided channels have changed drastically, Small eigenvalue changes, induced by large physical changes, are difficult to compute by correlated sampling.

The treatment of perturbations is particularly difficult when the perturbations are confined to small regions. Both the Matthes method and the method of complete correlation require that a substantial number of sample histories be tracked through the perturbed region. But if this region is small, then, in analog Monte Carlo, only a small fraction of the sample histories

will pass through it. It is clear that, in such cases, radical measures must be taken to enhance the density of sample neutrons near the perturbation. This might be done, for example, by conventional roulette and splitting. It is possible that biasing methods used by Steinberg and Kalos (22), in conjunction with their point estimation technique, may also be invoked (in place of splitting) to draw sample neutrons towards regions containing perturbations. In any case, as these regions decrease in size it becomes increasingly difficult to sense the perturbations, and the various effects which they induce.

In fixed source calculations, reaction rates in small regions are often computed by the adjoint method (25). Unfortunately, however, it is not a simple matter to adapt the adjoint method to reactivity computations. A Monte Carlo technique which incorporates the adjoint method into reactivity perturbation calculations has recently been developed by Bernnat (29). It is to be hoped that perturbation methods based on adjoint computations will be further elaborated and refined in the future.

At this point the Monte Carlo method is an essential tool of reactor analysis, essential in that it may often be feasible when all other methods fail. Yet the state-of-the-art today is far from satisfactory. Monte Carlo calculations are still generally very expensive. The theory of eigenvalue calculations is still primitive. Methods used for estimating confidence intervals need a good deal of improvement. Perturbation calculations are still difficult. In many respects, it seems deterministic methods are more highly developed and better understood than Monte Carlo methods. Perhaps it is time for a vigorous and concerted effort to extend the capabilities of Monte Carlo, since so much work on Monte Carlo remains to be done.

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